Spray-Combustion Modeling set-up at Argonne National Laboratory

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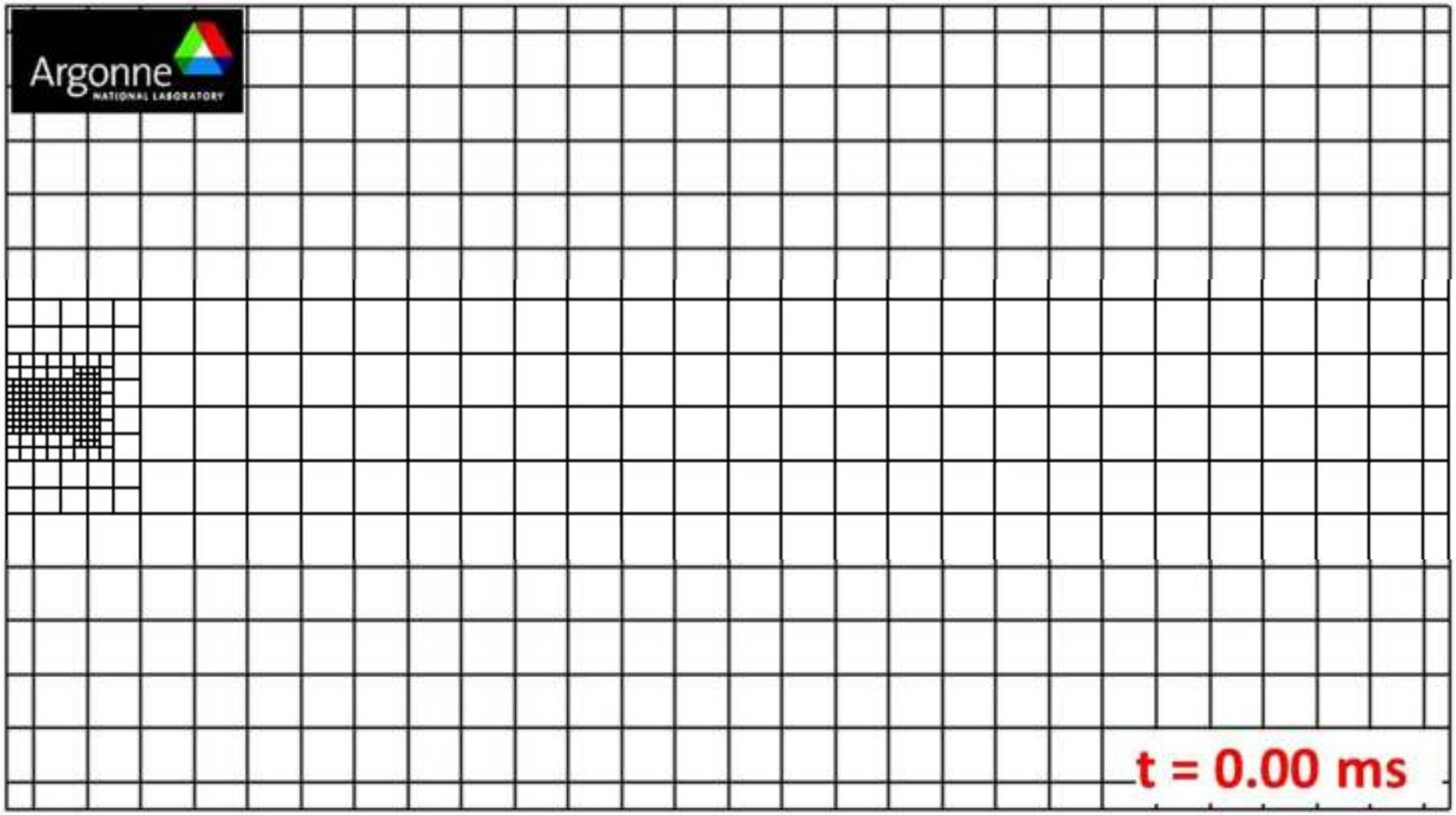
Engine Combustion Network Workshop - 1

Modeling Set-up

Modeling Tool	CONVERGE
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 2mm or 4mm Finest grid size: 0.125mm, 0.25mm, 0.5mm Gradient based AMR on the velocity and temperature fields. Fixed embedding in the near nozzle region to ensure the finest grid sizes
Total grid number	30K-40K for 0.5mm – RANS simulations (Non-reacting) 1.3 million for 0.125mm – LES case (Reacting) @ 3 ms
Parallelizability	Good scalability up to 48 processors

Turbulence and scalar transport model(s)	RNG k-ε, Standard k-ε, LES-Smagorinsky
Spray models	Breakup: KH-RT with breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model
Time step	Variable based on spray, evaporation, combustion processes
Turbulence-chemistry interactions model	Direct Integration of detailed chemistry well-mixed (no sub-grid model)
Time discretization scheme	PISO (Pressure Implicit with Splitting of Operators)
Chemistry acceleration	Analytical Jacobian

Adaptive Mesh Generation



Base Grid Size = 4 mm, Minimum Grid Size = 0.5 mm

LES Turbulence Model

The density weighted LES spatial filtering operation on the Navier-Stokes equation results in the filtered momentum equation:

$$\frac{\partial \overline{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \overline{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} - \frac{\partial \overline{\rho} T_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \tilde{u}_i}{\partial x_j}\right) - \overline{F}_i$$

where the LES sub-grid scale tensor: $T_{ij} = \left(\tilde{u_i u_j} - \tilde{u}_i \tilde{u}_j\right)$

is modeled using a Smagorinsky based model: $T_{ij} = -2C_s \Delta^2 \left|\overline{S}\right| \overline{S_{ij}} + \frac{1}{3}\delta_{ij} T_{kk}$

where $\left|\overline{S}\right| = \sqrt{2\overline{S_{ij}}\,\overline{S_{ij}}}$ $\quad \Delta = V_{cell}^{1/3}$ $\quad \overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right)$

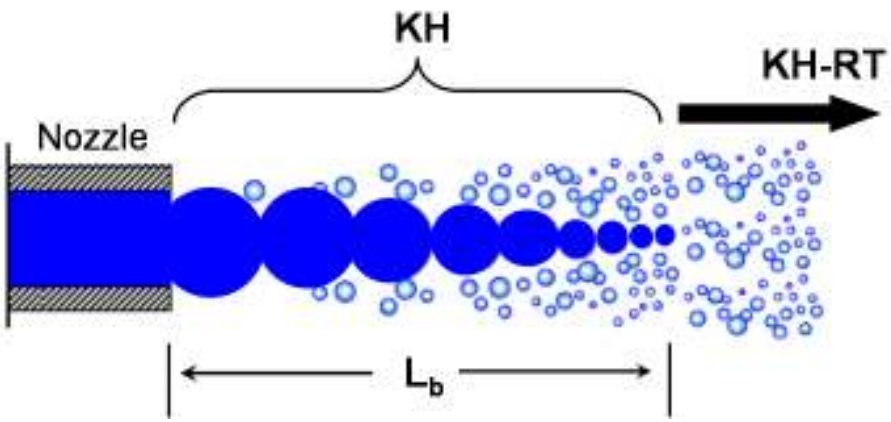
Sub-grid turbulent kinetic energy:

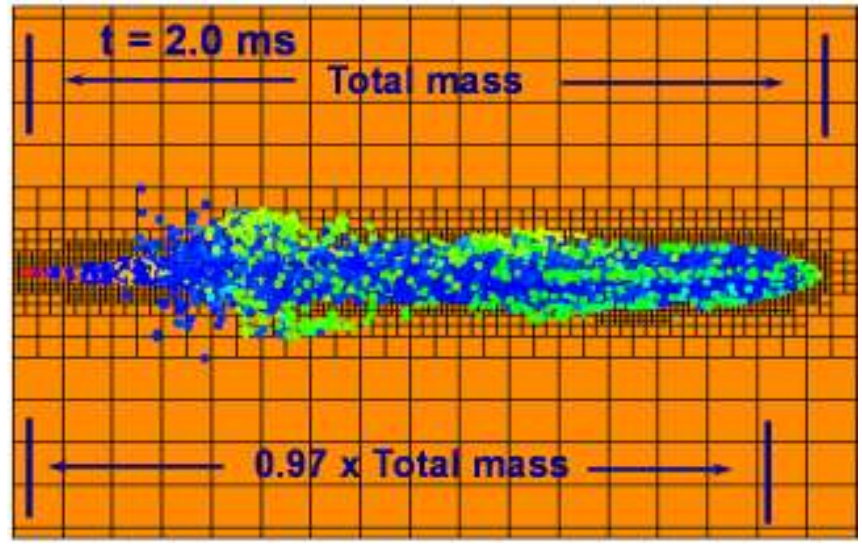
$$k \cong C_{les} \frac{\Delta^2}{24} \frac{\partial \overline{u_i}}{\partial x_j} \frac{\partial \overline{u_i}}{\partial x_j}$$

$C_s = 0.2$ **$C_{les} = 2.0$**

Definitions

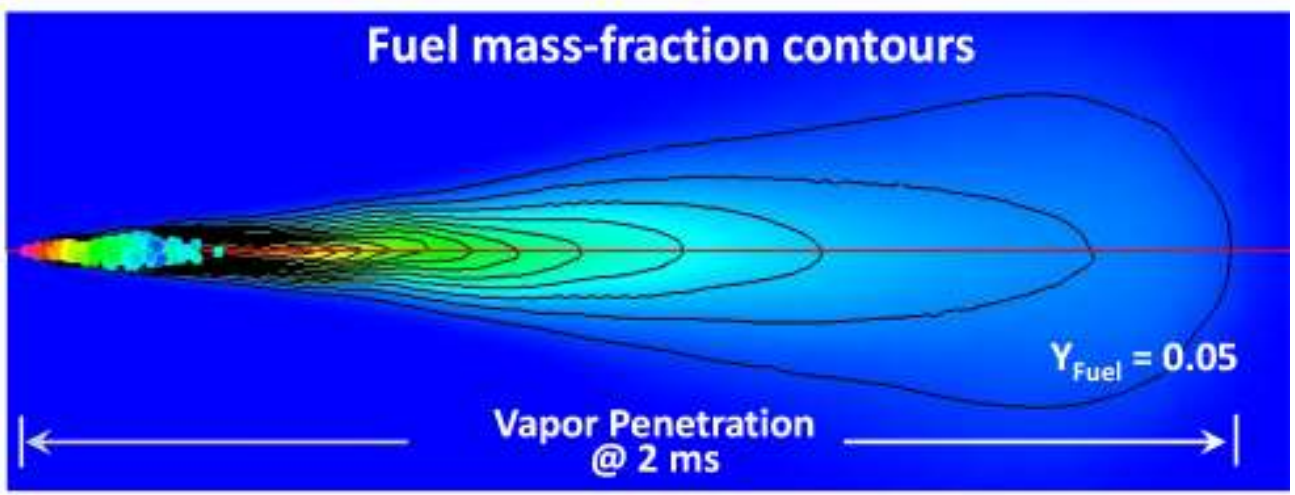
Break-up Length





Spray penetration @ 2 ms

Simulations with KH-ACT model not shown!

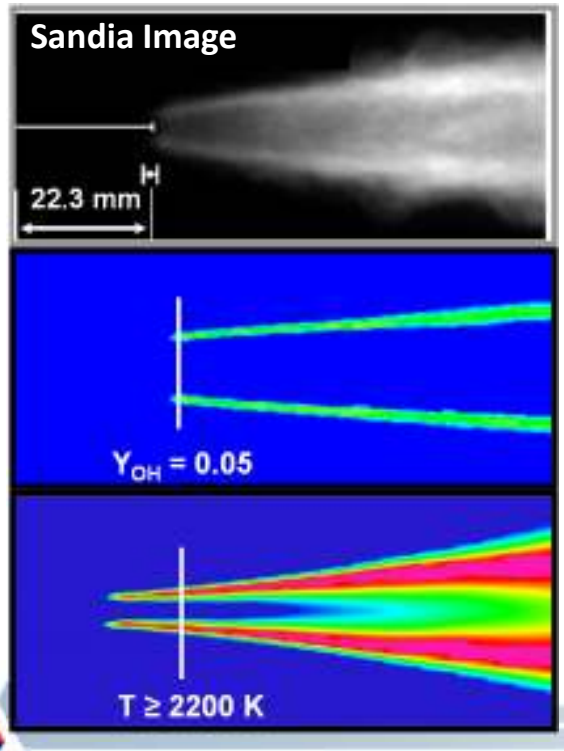


Spray and Combustion Set-up

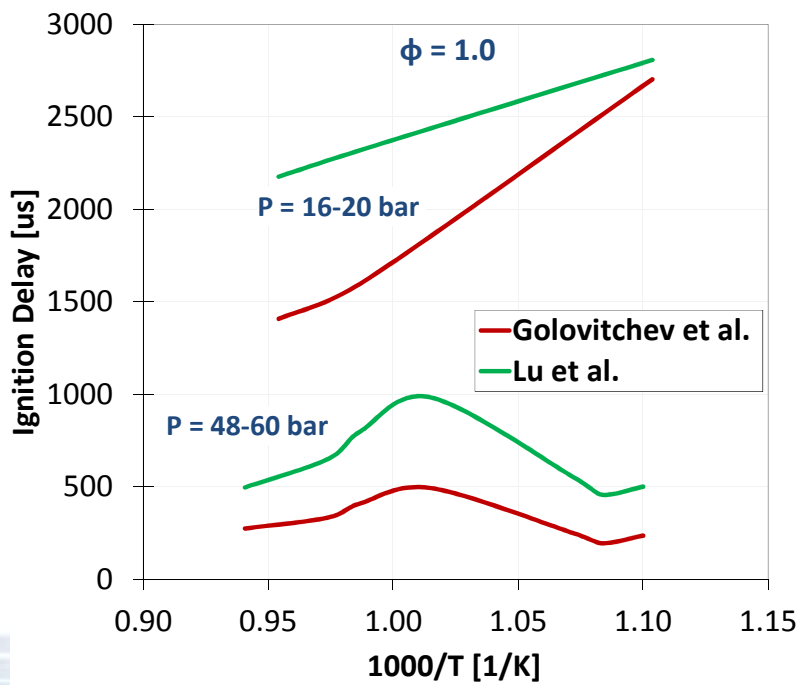
Chemical Kinetic Mechanism

1) 42 species, 283 reactions (**Golovitchev et al.**):
   V. I. Golovitchev, N. Nordin, R. Jarnicki, J. Chomiak. "3-D Diesel Spray Simulations Using a New Detailed Chemistry Turbulent Combustion Model," SAE Paper 2000-01-1891.
2) 68 species, 168 reactions (**Lu et al.**):
   Lu T. F., Law C.K., Yoo C.S., and Chen J.H., "Dynamic Stiffness Removal for Direct Numerical Simulations," Combustion and Flame, Vol. 156 No. 8 pp.1542-1551, 2009.

Lift-off length



Ignition delay: Ignition is said to occur when T ≥ 2000 K in a particular cell. Usually, coincides with appearance of OH.



Parametric Studies

- **Effect of turbulence model**
  1: RANS - Standard k-ε, RNG k-ε
  2: LES - Smagorinsky
- **Spray Structure**:
  1: Effect of grid-size: 0.5 mm, 1.0 mm, 2.0 mm
  2: Effect of time-step size

Non-reacting conditions for Spray A

- **Effect of Oxygen Concentration**:
  1: RANS-Golovitchev et al.(LOL, ID)
  2: RANS-Lu et al. (LOL, ID)
- **Effect of Ambient temperature**:
  1: RANS-Golovitchev et al. (LOL, ID)
  2: RANS-Lu et al. (LOL, ID)
  3: LES-Golovitchev et al. (LOL similar to RANS, Only ID)
- **Effect of Ambient density**:
  1: RANS-Golovitchev et al.(LOL, ID)
  2: RANS-Lu et al. (LOL, ID)

Reacting conditions for n-heptane

Note: Same set of spray constants were used for all parametric studies

(1) S. Som et al. , Combustion and Flame 2010
(2) S. Som, D.E. Longman & co-workers, ASME-ICE 2011